

A 3-D Hydrodynamic Dispersion Model for Modeling Tracer Transport in Geothermal Reservoirs

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Abstract

A 3-D hydrodynamic dispersion model for tracer transport is developed and implemented into the TOUGH2 EOS3 (T2R3D) module. The model formulation incorporates a full dispersion tensor, based on a 3-D velocity field with a 3-D, irregular grid in a heterogeneous geological system. Two different weighting schemes are proposed for spatial average of 3-D velocity fields and concentration gradients to evaluate the mass flux by dispersion and diffusion of a tracer or a radionuclide. This new module of the TOUGH2 code is designed to simulate processes of tracer/radionuclide transport using an irregular, 3-D integral finite difference grid in non-isothermal, three-dimensional, multiphase, porous/fractured subsurface systems. The numerical method for this transport module is based on the integral finite difference scheme, as in the TOUGH2 code. The major assumptions of the tracer transport module are: (a) a tracer or a radionuclide is present and transported only within the liquid phase, (b) transport mechanisms include molecular diffusion and hydrodynamic dispersion in the liquid phase in addition to advection, and (c) first order decay and linear adsorption on rock grains are taken into account. The tracer or radionuclide is introduced as an additional mass component into the standard TOUGH2 formulation, time is discretized fully implicitly, and non-linearities of the conservation equations are handled using the Newton/Raphson iteration. We have verified this transport module by comparison with results of a 2-D transport problem for which an analytical solution is available. In addition, a field application is described to demonstrate the use of the proposed model.

Introduction

It has been a challenge to simulate transport of a tracer in porous media using a general 3-D, irregular grid with a numerical method. One of the difficulties in solving advection-diffusion type transport equations is how to approximate the dispersion tensor in order to estimate the dispersive terms of mass transport accurately. Most of numerical modeling approaches in the literature (e.g., Huyakorn and Pinder, 1983; Oldenburg and Pruess, 1997) use numerical schemes that are based on regular grids with finite element or finite difference spatial discretization. However, it may be impractical to use a regular grid in conducting modeling studies in many field applications. One of such examples is the site-scale modeling study on tracer or radionuclide transport at Yucca Mountain, Nevada, a potential underground radioactive waste repository, in which a irregular 3-D grid has to be used (Bodvarsson et al., 1997) for the large, complex geological system there.

We have developed a 3-D hydrodynamic dispersion model for tracer transport and implemented the model into the TOUGH2 code (Pruess, 1991). The model formulation incorporates a full dispersion tensor, based on a 3-D velocity field with a 3-D, irregular, integral finite difference grid in a heterogeneous geological system. Two different weighting schemes are proposed for spatially averaging 3-D fluid flow velocity and tracer concentration gradients. It takes account of the physical processes of tracer transport in a non-isothermal, multi-phase, multi-dimensional flow environment in the subsurface. The treatment of water, air and heat flow is identical to that of the standard TOUGH2 module (Pruess, 1991). The major assumptions for the tracer transport module(T2R3D): include (a) a tracer exists and is transported only within the liquid phase; (b) transport mechanisms considered are molecular diffusion and hydrodynamic dispersion in the liquid phase in addition to advection terms; (c) first order decay is taken into account; and (d) adsorption of a tracer on the rock matrix is described by an equilibrium isotherm with a constant distribution coefficient.

In this paper, we will present the model formulation proposed for determining 3-D hydrodynamic dispersion coefficients with irregular grids. Also a verification sample is given in which the transport module is examined with results of a 2-D transport problem for which an analytical solution is available. The proposed model has been used in the field studies of tracer and radionuclide transport at the Yucca Mountain site.

Model Formulation

The basic mass and thermal energy balance equations solved by T2R3D are the same in form as those by the standard TOUGH2 module (Pruess, 1991). The difference is that T2R3D introduces an additional component, a tracer/radionuclide. Therefore, the total number of mass components in T2R3D is three, with component #1 = water, #2 = air, and #3 = tracer or radionuclide. In terms of the integral formulation, the conservation of mass and thermal energy is described (Pruess, 1991) by

$$\frac{d}{dt} \int_{V_n} \mathbf{M}^{(\kappa)} dV = \int_{\Gamma_n} \mathbf{F}^{(\kappa)} \cdot \mathbf{n} d\Gamma + \int_{V_n} q^{(\kappa)} dV \quad (1)$$

The integration here is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_n . The quantity \mathbf{M} appearing in the accumulation term denotes mass or energy per unit volume, with $\kappa = 1$ (air), $\kappa = 2$ (water) and $\kappa = 3$ (tracer) labeling the mass components, and $\kappa = 4$ for “heat component. \mathbf{F} is a general “flow” term including Darcy’s flow, mass advection/diffusion and heat convection/conduction transfer, and q is a sink/source term.

The general form of the mass accumulation term is

$$\mathbf{M}^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} X_{\beta}^{(\kappa)} \quad (2)$$

The total mass of component κ is obtained by summing over all fluid phases $\beta = 1$ (gas) and 2 (liquid). S_β is the saturation (volume fraction) of phase β , ρ_β is density of phase β , and $X_\beta^{(\kappa)}$ is the mass fraction of component κ present in phase β .

The heat accumulation term is defined as

$$M^{(4)} = \phi \sum_{\beta=1}^2 S_\beta \rho_\beta u_\beta + (1-\phi) \rho_R C_R T \quad (3)$$

where u_β is internal energy of fluid phase β , C_R is specific heat of rock, ρ_R is density of rock and T is reservoir temperature.

The mass flux term of components is a sum over the phases

$$\mathbf{F}^{(\kappa)} = \sum_{\beta=1}^{NPH} X_\beta^{(\kappa)} \mathbf{F}_\beta \quad (4)$$

for $\kappa = 1, 2$ and 3. Individual phase mass fluxes are given by a multi-phase version of Darcy's law:

$$\mathbf{F}_\beta = -k \frac{k_{r\beta}}{\mu_\beta} \rho_\beta (P_\beta - \rho_\beta \mathbf{g}) \quad (5)$$

Here k tensor is absolute permeability tensor, $k_{r\beta}$ is relative permeability of phase β , μ_β is viscosity of phase β , and

$$P_\beta = P + P_{c,\beta} \quad (6)$$

is the pressure in phase β , which is the sum of the pressure P of a reference phase, and the capillary pressure ($P_{c\beta}$) of phase β relative to the reference phase. \mathbf{g} denotes the vector of gravitational acceleration.

The heat flux is given by

$$\mathbf{F}^{(4)} = -K_{th} \nabla T + \sum_{\beta=1}^2 h_\beta \mathbf{F}_\beta \quad (7)$$

where K_{th} is thermal conductivity of the formation, h_β is the specific enthalpy of phase β .

The mass flux term for the tracer/radionuclide component in the liquid phase is described by

$$\mathbf{F}^{(3)} = \mathbf{F}_A^{(3)} + \mathbf{F}_D^{(3)} \quad (8)$$

where the first term on the right-hand side is mass flux by advection, defined as

$$\mathbf{F}_A^{(3)} = X_\beta^{(3)} \mathbf{F}_\beta \quad (9)$$

The phase mass flux \mathbf{F}_β (β = liquid) in (9) is given in Equation (5) by Darcy's law, and $X_\beta^{(3)}$ is the mass fraction of a tracer/radionuclide in the liquid phase.

The second term on the right-hand side of (9) is the dispersive and diffusive mass flux, defined as

$$\mathbf{F}_D^{(3)} = -\rho_\beta \bar{D} \bullet \nabla X_\beta^{(3)} \quad (\beta=\text{liquid}) \quad (10)$$

where \bar{D} is the combined diffusion-dispersion tensor accounting for both molecular diffusion and hydrodynamic dispersion. We have incorporated a general dispersion model for 3-D tracer transport into the T2R3D code (Scheidegger, 1961),

$$\bar{D} = \alpha_T |\mathbf{v}_\beta| \delta_{ij} + (\alpha_L - \alpha_T) \frac{\mathbf{v}_\beta \mathbf{v}_\beta}{|\mathbf{v}_\beta|} + \phi S_\beta \tau d_m \delta_{ij} \quad (\beta=\text{liquid}) \quad (11)$$

where α_T and α_L are the transverse and longitudinal dispersivities, respectively; \mathbf{v}_β is the Darcy's velocity vector of phase β ; τ is the tortuosity of the medium; d_m is the molecular diffusion coefficient in phase β ; and δ_{ij} is the Kroneker delta function. ($\delta_{ij}=1$ for $i=j$, and $\delta_{ij}=0$ for $i \neq j$)

The treatment of adsorption and first-order decay effects in T2R3D follows the work by Oldenburg and Pruess (1995) using the integral finite difference formulation. The mass accumulation term including adsorbed tracer/radionuclide on the rock matrix is

$$M^{(\kappa)} = \phi S_\beta \rho_\beta X_\beta^{(\kappa)} + (1 - \phi) \rho_R \rho_\beta X_\beta^{(\kappa)} K_d \quad (12)$$

where K_d is the distribution coefficient of the tracer/radionuclide partitioning between the aqueous phase and rock grains.

The first-order decay of a tracer/radionuclide is handled using the integral-finite-difference-discretized equation (Pruess, 1991; Oldenburg and Pruess, 1995),

$$M_n^{k,k+1} (1 + \lambda_\kappa \Delta t) - M_n^{k,k} = \frac{\Delta t}{V_n} \left\{ \sum_m A_{nm} F_{nm}^{k,k+1} + V_n q_n^{k,k+1} \right\} \quad (13)$$

where subscript n denotes a grid block n ; λ_κ is the radioactive decay constant of the radionuclide (component $\kappa=3$), and is defined as

$$\lambda_\kappa = \frac{\ln(2)}{T_{1/2}} \quad (14)$$

with $T_{1/2}$ being the half-life of the tracer/radionuclide component.

One of the key issues in implementing the general 3-D dispersion tensor of (11) into T2R3D is how to average velocity fields for determining the dispersion tensor. We have adopted a spatial and harmonic weighting scheme to evaluate a velocity vector at the interfaces between element blocks, as shown in Figure 1. In Figure 1, V_m and V_n are the volume blocks m (neighboring) and n . A_{nm} is the area of the interface between the two blocks, D_m and D_n are the distances from the interface to each block's center, and \mathbf{v}_m and \mathbf{v}_n are the fluid velocities at the center of each block, while \mathbf{v} is the velocity of liquid at the interface between blocks. \mathbf{n} is the unit vector at the connection between the two blocks along connection nm , with a component n_i ($i=x,y,z$), or directional cosines, in the x -, y -, or z -direction, respectively. Also the positive direction of \mathbf{n} is defined as the direction from the block center of V_m toward the block center of V_n , as shown in Figure 1. In addition, all three velocity vectors, \mathbf{v}_n , \mathbf{v}_m , and \mathbf{v} , and the connection-direction vector, \mathbf{n} , are relative to the global coordinate system of (x, y, z) .

First we need to convert the local fluxes along connections in the local coordinates to a velocity vector, \mathbf{v}_n , in the system of global coordinates (x, y, z) at the block center for each block of the grid. The averaging or weighting scheme used is called “*projected area weighting method*”, in this method a velocity component, $v_{n,i}$, of the vector \mathbf{v}_n is determined by the vectorial summation of the flow components of all local connection vectors in the same direction, weighted by the projected area in that direction,

$$v_{n,i} = \frac{\sum_m (A_{nm} |n_i|) (v_{nm} n_i)}{\sum_m (A_{nm} |n_i|)} \quad (i=x,y,z) \quad (15)$$

where m is the total number of connections between element V_n and all its neighboring elements V_m , and v_{nm} is the flux along connection nm in the local coordinate system. In Equation (15), the term, $(A_{nm} |n_i|)$, is the projected area of the interface A_{nm} on to the direction i ($i=x,y,z$) of the global coordinate system, and $(v_{nm} n_i)$ gives the velocity component in the direction i of the global coordinate system, contributed by the local flux v_{nm} between blocks V_n and V_m . Also it should be mentioned that the absolute value for the directional cosines, n_i , are used for evaluating the projected area in Equation (15), because only the positive areal values are needed for the weighting scheme.

The velocity vector \mathbf{v} at the interface of elements n and m is evaluated by harmonic weighting by the distances to the interface using the velocities at the block centers of the two elements,

$$\frac{D_n + D_m}{V_i} = \frac{D_n}{V_{n,i}} + \frac{D_m}{V_{m,i}} \quad (i= x, y, z) \quad (16)$$

for its component v_i . Harmonic weighting is here used because it preserves total transit time for solute transport travelling between the two blocks.

The fluid flow velocity \mathbf{v} or \mathbf{v}_β , determined by equation (16), is used in Equation (11) to evaluate the dispersion tensor along the connection of the two elements of m and n.

On the other hand, the concentration or mass fraction gradient of the tracer/radionuclide is evaluated, based on the “*interface area weighting scheme*”. The mass fraction gradient, a vector, at element n is given by an areal weighting scheme:

$$\nabla \mathbf{X}_n^{(\kappa)} = \frac{\sum_m A_{nm} \nabla \mathbf{X}_{nm}^{(\kappa)}}{\sum_m A_{nm}} \quad (\kappa=3) \quad (17)$$

where $\nabla \mathbf{X}_{nm}^{(\kappa)}$ is the mass fraction gradient of a tracer/radionuclide along connection nm in the global coordinate system, evaluated by

$$\nabla \mathbf{X}_{nm}^{(\kappa)} = (n_x \Delta X_{nm}^{(\kappa)}, n_y \Delta X_{nm}^{(\kappa)}, n_z \Delta X_{nm}^{(\kappa)}) \quad (18)$$

with

$$\Delta X_{nm}^{(\kappa)} = \frac{X_m^{(\kappa)} - X_n^{(\kappa)}}{D_m + D_n} \quad (19)$$

The reason behind the interface area weighting method is that the dispersive fluxes between all the connected elements are directly proportional to the interface areas, therefore a local concentration gradient with a larger connected interface area should take more weight in the resultant gradient at the block.

Once two mass fraction gradients at the two blocks m and n are determined, the mass fraction gradient ∇X at the interface between two blocks is evaluated by a linear interpolation for its component i (i=x, y, z),

$$\nabla X_i^{(\kappa)} = \frac{D_m}{D_m + D_n} \nabla X_{n,i}^{(\kappa)} + \frac{D_n}{D_m + D_n} \nabla X_{m,i}^{(\kappa)} \quad (20)$$

This mass fraction gradient of (20) will be used to calculate the total diffusive and dispersive mass flux of a tracer/radionuclide along the connection of the two elements.

The net mass flux of diffusion and dispersion of a tracer/radionuclide along the connection of elements V_n and V_m is determined by

$$F_{nm}^{(\kappa)} = \mathbf{n} \cdot \mathbf{F}_D^{(\kappa)} = -\mathbf{n} \cdot [\rho_\beta \bar{D} \cdot \nabla X_\beta^{(\kappa)}] \quad (21)$$

Finally, the diffusive and dispersive flux of Equation (21) is added to the total flux term of Equation (8) for the tracer/radionuclide component along the connection of the two elements, which contributes the flow term for the tracer/radionuclide component in the conservation

equation of (1) or (13). It should be mentioned that incorporation of (21) into (13) gives rise to extra terms in the Jacobian matrix in addition to those contributed by only two advectively-connected blocks. These additional Jacobian terms have been ignored in the present model, because so far we have not observed problems with convergence rates using the incomplete Jacobian for weakly-coupled tracer transport problems. However, convergence rates may deteriorate in strongly-coupled or large dispersive transport situations, even though converged solutions are still correct.

Verification Example

In order to examine the accuracy of approximation of the formulation discussed above in handling transport in a multi-dimensional domain with hydrodynamic dispersion and molecular diffusion effects, we have checked the numerical solutions against several analytical solutions (Wu et al., 1996). One of those verification samples is discussed in this section and the problem is similar to the one used by Oldenburg and Pruess (1993). The problem concerns two-dimensional transport of a radionuclide in a homogenous isotropic, saturated porous medium. The model domain is rectangular, as shown in Figure 2. There is a steady-state, one-dimensional flow field along the x-direction with pore velocity of 0.1 m/day in the domain. A tracer/radionuclide is introduced along a line source of length of 0.5 meter at $x=0$ with a constant concentration. Transport starts at $t=0$ from the line source by advection, hydraulic dispersion and diffusion. An analytical solution for this problem is provided by Javandel et al. (1984) along with a code for calculating the 2-D concentrations. The analytical solution is used here to verify the T2R3D numerical solution.

The T2R3D solution of this problem is accomplished by specifying on both the upstream boundary ($x=0$) and downstream boundary ($x=6$ m) a constant pressure, which gives rise to a steady-state flow field of 0.1 m/day flow velocity. Also, in the T2R3D simulation, a uniform grid spacing was used for both x and y directions with $\Delta x = \Delta y = 0.1$ m. The system is kept at single liquid-phase and isothermal conditions. Air mass fraction is set to zero and a constant temperature of 25 °C is specified. Also no decay or adsorption effects are included in the simulation. The properties used in the comparison study are: porosity $\phi = 1$, tortuosity $\tau = 1$, molecular diffusion coefficient $D_m = 1.0 \times 10^{-10}$ m²/s, longitudinal dispersivity α_L is 0.1 m, and transverse dispersivity α_T is 0.025 m. The liquid properties are internally generated by the code. The initial and boundary conditions for the radionuclide are: initially there is no radionuclide in the system; $X^{\text{radionuclide}} = 1.0 \times 10^{-5}$ along the 0.5 m line source; and $X^{\text{radionuclide}} = 0$ at the downstream boundary ($x=6$ m) at all times.

Figure 1 Schematic of spatial averaging scheme for velocity fields in the integral finite difference method.

Figure 2 Schematic of the 2-D domain the 2-D radionuclide transport problem showing the velocity field and three cross sections for comparisons with the simulations results.

Figure 3 Comparison of radionuclide concentration profiles along cross section (A-A') from analytical and numerical solutions at $t=20$ days.

Figure 4 Comparison of radionuclide concentration profiles along cross section (B-B') from analytical and numerical solutions at $t=20$ days.

Figure 5 Comparison of radionuclide concentration profiles along cross section (C-C') from analytical and numerical solutions at $t=20$ days.

Comparison of the normalized radionuclide concentrations along the three cross-sections of the rock column from the T2R3D and the analytical solution are shown in Figures 3, 4, and 5 for time = 20 days, respectively. The figures indicate that the T2R3D simulated concentration profiles in the two-dimensional domain are in good agreement with the analytical solution. Figure 3 shows the radionuclide profile at $y=0.15$ m (cross section A-A' in Figure 2), indicating an excellent agreement between the two solutions along this cross section. Figure 4 shows the concentration profile at $y = 0.75$ m, just below the line source which extends from $y = 0$ to $y = 0.5$ m, and this figure displays both longitudinal and transverse dispersion effects. As can be seen in Figure 4, the comparison is good even though small numerical errors are introduced in the numerical solution. Figure 5 gives the comparison of concentration profiles along the transverse direction (C-C') at $x = 2$ m, indicating an excellent agreement between the analytical and numerical solutions at this location.

Field Application

A field application example of the T2R3D module is provided in this section, and the problem concerns the unsaturated zone transport of environmental isotopic tracers at Yucca Mountain (Fairley and Wu, 1997). Field studies of environmental isotopic tracers at Yucca Mountain have revealed the presence of fast pathways for moisture flow from the land surface to the proposed repository horizon (several hundreds of meters deep), and water traveling time is estimated as less than 40 years because of detection of significant quantities of tritium, ^{36}Cl , or ^{99}Tc (Fabryka-Martin et al., 1996; Yang et al., 1996). Here T2R3D is used to attempt to quantify when pathways form, and under what conditions they may be detectable. The tracer data, the $^{36}\text{Cl}/\text{Cl}$ ratios, are the most complete isotopic measurements at the site and were chosen for the present study.

A two-dimensional vertical cross section, irregular grid was generated to model the tracer transport, and the detailed information of the input parameters, model grid and boundary conditions were discussed by Fairley and Wu (1997). The top boundary of the 2-D model is the land surface and the bottom is on the regional water table. The entire unsaturated zone formation consists of fractured/matrix rocks, and the fracture/matrix interactions were treated using the dual-permeability modeling approach. Both steady state and transient simulations have been conducted to look at the tracer transport phenomena at the site, and are shown Figures 6 and 7. Figure 6 shows the steady-state distributions of ^{36}Cl concentrations at the mountain, indicating a relative uniform downward penetration of the chloride. Figure 7 gives the results of the transient simulations, and shows a much deep travel distance or a fast pathway at one location. This location corresponds to a fault structure at the site. Model simulation results indicate that fast pathways probably arise from rapidly transient infiltration

events, and are associated with structural discontinuities of one of the hydrogeologic units of the formation. Fast flow pathways at the site are likely to carry only a small fraction of the total percolation flux.

Figure 6 Steady state simulations of ^{36}Cl isotope transport in the unsaturated zone of Yucca Mountain.

Figure 7 Transient simulations of ^{36}Cl isotope transport in the unsaturated zone of Yucca Mountain.

Summary

We have presented a 3-D hydrodynamic dispersion model for tracer transport and implemented it into the TOUGH2 code as a new (T2R3D) module. The model formulation incorporates a full dispersion tensor using a 3-D, irregular grid in a heterogeneous geological system. Two physically-based weighting schemes were proposed for spatial average of 3-D velocity fields and concentration gradients, respectively, to evaluate the mass flux by dispersion and diffusion of a tracer or a radionuclide. The new transport module of the TOUGH2 code has been verified by comparison with results of a 2-D analytical solution. Application of the new TOUGH2 module to the site-scale modeling studies of environmental isotopic tracer transport at Yucca Mountain has provided some insights into moisture flow and tracer transport at the site.

Acknowledgment

We thank Curt Oldenburg and Jerry Fairley for help in this work. Thanks are also due to H. H. Liu and K. Huang for reviewing the manuscript. This work was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Division. This work was also supported in part by the Director, Office of Civilian Radioactive Waste Management, U. S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems Inc. and the Ernest Orlando Lawrence National Laboratory. The support is provided to Berkeley Lab through the U. S. Department of Energy Contract No. DE-AC03-76SF00098.

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